Large-Scale Time-Dependent Schrödinger Equation Solver

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The combination of cold (neutral) atom technology with well-established photo-ionization techniques opens up a new territory for experimental exploration. The ionization of a fraction of the cold atoms in a Bose-Einstein condensate (BEC) creates impurity particles (ions and electrons) that are electrically charged and, hence, interact much more strongly and over much larger distances than the initial neutral atoms. If a large number of such charged particles are created, the strong interparticle correlations quickly heat and/or destroy the cold atom system. Alternatively, a BEC with only a few ions would survive for a longer time and such a system could provide an interesting laboratory for studying the dynamics and phase coherence of the BEC. A useful description of the few-ion BEC treats the ions as classical impurity particles embedded in a superfluid. As in the condensed helium experiments that controlled the motion of ring vortices by steering electrons that were trapped by the individual ring vortices, the charge of an impurity atom, easily manipulated by an external electric field, could provide a handle to probe and control superfluid dynamics.

The electric field of the charge polarizes the neutral BEC atoms and the interaction of the resulting dipole with electric field results in a mutual attraction that varies as the inverse fourth power of the ion-atom distance. One notable speculation suggested that the resulting polarization potential could capture hundreds of neutral atoms into a single long-range orbit surrounding the ionic impurity to make a giant, mesoscopic molecule. Our simulation of the dynamics of the BEC responding to the sudden appearance of the polarization potential indicates that the survival and observation of such a long-range molecule is highly unlikely. The BEC-superfluid responds by initially rushing towards the suddenly created center of attraction, until the local density increase near the ion position gives a positive pressure that causes the superfluid flow to reverse itself. The rather violent flow dynamics with oscillatory density profiles that vary rapidly would rapidly destroy any long-range range molecule. On the other hand, the dynamics of the BEC-response to a highly singular potential provides an ideal test case to understand the BEC-dynamics and its effect on the coherence of the BEC. This violent dynamics driven by a highly singular potential also presents a significant challenge to simulate numerically as one needs to follow the evolution of the BEC over a long time scale and more importantly excessively large distances.

To address this issue, we developed a highly parallel 3D time-dependent Schrödinger equation solver. The parallel algorithm developed solves the 3D time-dependent Schrödinger equation using the split operator method. In this formulation, the wave function is propagated in time by the successive application of two different exponential operators, one containing the kinetic and the other the potential part of the Hamiltonian. This method assumes that the Hamiltonian is constant between two time steps. Application of a finite difference formula to the kinetic part leads to the real-space product algorithm where the solution of the time-dependent Schrödinger equation is reduced to a series of matrix-vector multiplications. This method has been widely used to solve various problems involving the time-dependent Schrödinger equation but, to our knowledge, a parallel algorithm has not been explicitly elaborated.

In the parallel scheme developed, we aimed at distributing the wave function uniformly over the total number of processors. This approach is the most attractive as, in such a scheme, each processor contains and propagates only a part of the wave functions. This leads to a fully distributed memory scheme where the total wave function is never accumulated on a single processor. While this approach can be applied to each dimension

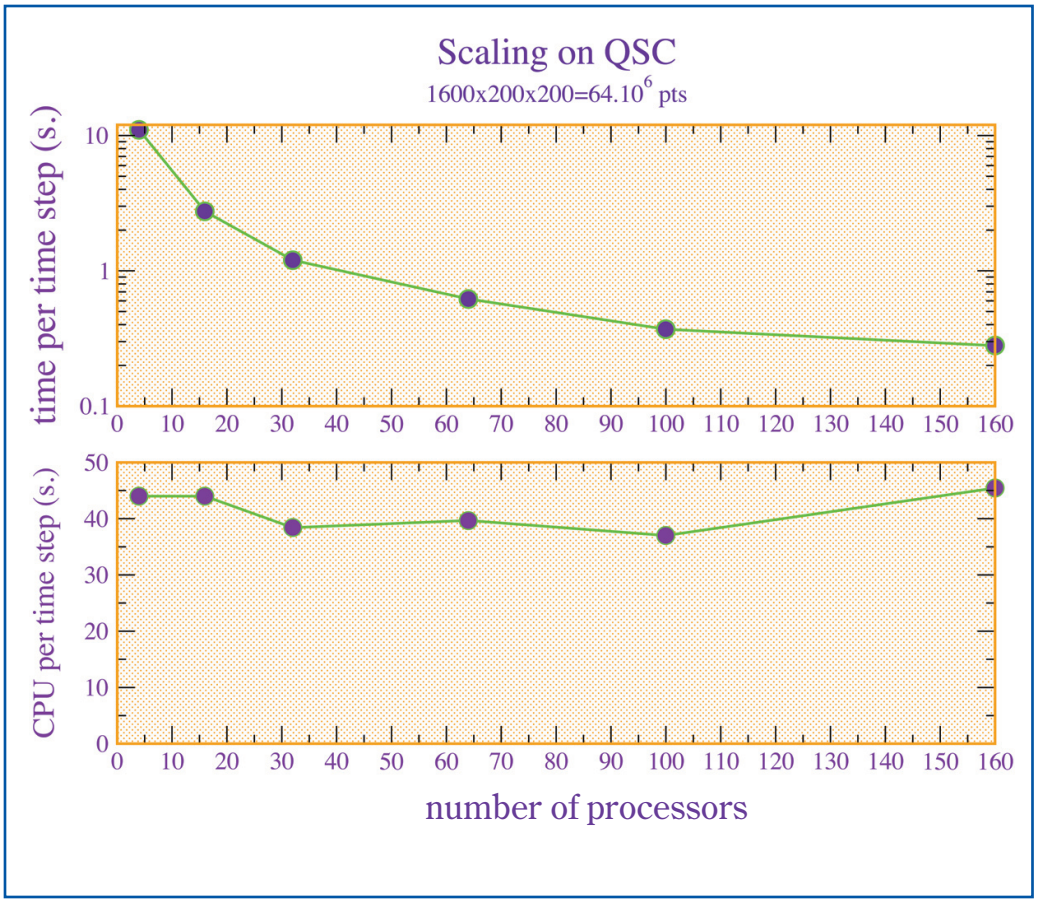

Figure 1— Scaling on the Q machine for the propagation of a BEC on a 64×10^6-point grid.

without difficulties, we made the choice of distributing the wave function along a single dimension. In elaborating such an approach, the main difficulty to overcome resides in the evaluation of the kinetic energy operator. In contrast to the potential energy operator, the application of the kinetic energy operator involves the knowledge of the previous time step wave function at several grid points. The number of grid points needed is defined by the order of the finite difference scheme used. Using the standard message-passing library MPI, we developed an efficient scheme to exchange information between processors. The efficiency of the algorithm developed is illustrated in Fig. 1 where we obtained a perfect scaling up to 160 processors on the QSC machine for the propagation of a BEC on a 64×10^6-point grid.